Parallel Iterative Solvers with the Selective Blocking Preconditioning for Simulations of Fault-Zone Contact

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Abstract

Iterative solver with preconditioning is the most powerful choice for large-scale scientific computation, especially for the parallel computing. In nonlinear problems such as contact simulations for geophysics, the condition numbers of the coefficient matrices are usually large due to special constraint conditions. The result is slow convergence of the iterative solver. In this study, a new preconditioning method, called *selective blocking* was developed along with special partitioning method for parallel computing on the GeoFEM platform. This newly developed method provides robust and smooth convergence in 3D solid mechanics simulations for geophysics with contact conditions performed on a Hitachi SR2201 parallel computer with 128 processing elements.

1. Introduction

One of the most important applications of GeoFEM [1] is simulation of ground motion. Stress accumulation on plate boundaries (faults) is very important in estimating the earthquake generation cycle (Fig. 1).

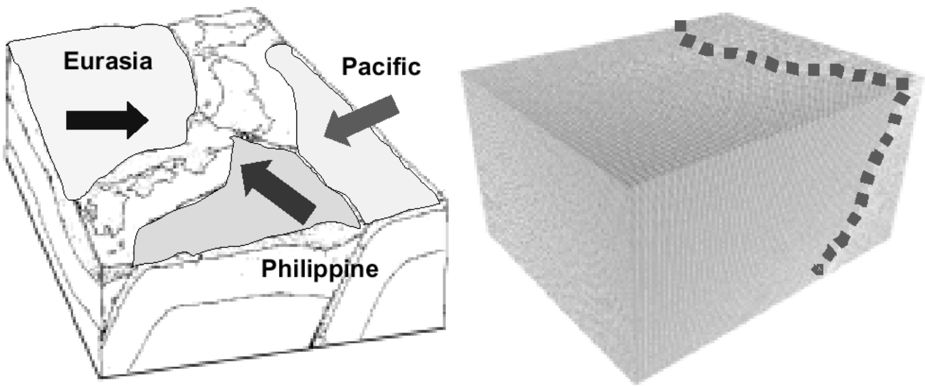


Fig. 1 Plate boundaries (faults) around Japanese Islands and an example of the finite element model (6,156 elements, 7,220 nodes, 21,660 DOF, 840km×1020km×600km region)

In ground motion simulations, material, geometric and boundary nonlinearity should be considered. Boundary nonlinearity due to *fault-zone contact* is the most critical. In GeoFEM, the augmented Lagrange method (ALM) and penalty method are implemented, and a large penalty number λ is introduced for constraint conditions around faults [2]. This penalty number provides ill-conditioned coefficient matrices for linear solvers.

In this paper, *selective blocking* was implemented to block ICCG solvers for fault-zone contact simulation. This method provides robust and efficient convergence. Moreover, a special partitioning method for parallel computation was developed in order to eliminate *edge-cuts* in contact groups. Parallel performance of this method was demonstrated on a Hitachi SR2201 parallel computer with 128 processing elements (PEs). In this paper, we will provide a brief overview of the parallel iterative solvers in GeoFEM, outline the *selective blocking* along with special partitioning, and show some examples.

2. Selective Blocking

Table 1 shows the results of the convergence of one certain Newton-Raphson iteration during contact simulation by various types of preconditioned CG methods for the finite element application (6,156 elements, 7,220 nodes, 21,660 DOF, 840km×1020km×600km region). This was computed with a single processor. λ is the normalized penalty number divided by Young's modulus (E). Coefficient matrices are symmetric for 3D elastic contact problems if there is no friction on fault surfaces. The first two items of Table 1 show the results by GeoFEM's original scalar CG solver preconditioned by diagonal scaling and IC with no fill-in. In GeoFEM's original scalar solvers, all DOF are treated independently. In these cases, the iterative solver converges fast if $\lambda=10^0$, but does not converge at all if $\lambda=10^6$.

The typical remedies using an IC/ILU type of preconditioning method for ill-conditioned matrices are as follows:

- Blocking
- Deep Fill-in
- Reordering.

First of all, 3×3 block operation was introduced for 3D solid mechanics. In 3D solid mechanics problems, there are three DOF on each finite-element node. Full LU factorization is introduced in this 3×3 block. Thus, by using a block IC preconditioning (BIC), three DOF on the same finite-element node can be treated in a more simultaneous manner than by using the original *scalar* IC preconditioning in GeoFEM.

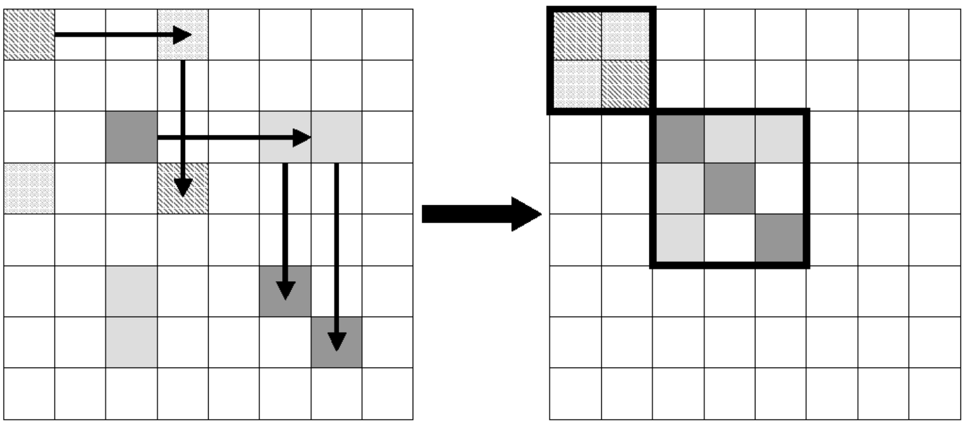
Another remedy for ill-conditioned matrices – *deep fill-in* – applies a level of fill-in to block IC preconditioning (BIC(n), where n is the level of fill-in). Besides deep fill-in, a special method named *selective blocking* has also been developed for contact problems. In the *selective blocking* method, strongly coupled finite-element nodes are put into the same large block *(selective block* or *super* node) and reordered according to the blocking. Full LU factorization is applied in the selective blocks of a matrix block of size (3×NB) × (3×NB), where NB is the number of finite-element nodes in the selective blocks, as shown in Fig.2. In contact problems, the *selecting blocking* procedure can be applied to the finite-element nodes in each contact group coupled through penalty constraints. Thus, coupled finite-element nodes in contact groups can be treated in a simultaneous manner during preconditioing procedure.

By introducing the 3×3 block, CG solver preconditioned by block IC with no fill-in (BIC(0)) converges even when λ is as large as 10^6 (Table 1). *Deep fill-in* options provide faster convergence but the SB-BIC(0) (BIC(0) preconditioning combined with the *selective blocking* reordering) shows the best performance (Table 1). In SB-BIC(0), no *inter-block* fill-in has been considered. Especially in the case where $\lambda = 10^{10}$, SB-BIC(0) provides the fastest convergence, while BIC(1) stagnates.

Table 1. Iterations/CPU time (includes factorization) until convergence ($\varepsilon = 10^{-8}$) on a single PE COMPAQ Alpha 21164/600MHz by preconditioned CG for the 3D elastic fault-zone contact problem in Figure1 (21,660 DOF).

Preconditioning	λ	Iter #	sec.
Diagonal	10^0	340	19.1
Scaling	10^6	No Conv.	N/A
IC(0)	10^0	85	8.9
(Scalar Type)	10^6	No Conv.	N/A
BIC(0)	10^0	82	8.8
	10^6	1,108	116.8
BIC(1)	10^0	44	9.4
	10^6	94	17.9
	10^{10}	No Conv.	N/A
BIC(2)	10^0	32	12.2
	10^6	33	13.0
	10^{10}	1,798	450.9
SB-BIC(0)	10^0	78	9.4
	10^6	77	9.4
	10^{10}	141	18.0

BIC(n): Block IC with n-level fill-in, **SB-BIC(0)**: BIC(0) with the selective blocking reordering.



(a) (b)

Fig. 2 Procedure of the *selective blocking* : Strongly coupled elements are put into the same *selective bloc*k. (a) searching for strongly coupled components and (b) reordering and selective blocking.

3. Strategy for Parallel Performance

Localized ILU/IC [1] is an efficient parallel preconditioning method, but it is not necessarily robust for ill-conditioned problems. Table 3 shows the results by parallel CG solvers with localized preconditioning on a 4 PE workstation cluster using distributed matrices created by k-way METIS [6], for the problem described in Fig.1 and Table 2. According to the results, the number of iterations for convergence increases by a factor of 10 in $\lambda = 10^6, 10^{10}$ cases. This is because the *edge-cuts* occur at inter-partition boundary edges that are included in contact groups [4].

In order to eliminate these edge-cuts, a partitioning technique has been developed so that all nodes which belong to the same contact groups are on the same partitions. In GeoFEM, there are several types of special elements for contact problems (types 411, 412, 421, 422, 511, 512, 521 and 522) [1]. Nodes included in the same elements of these types are connected through penalty constraints and form a contact group. In the new partitioning method, the partitioning process is executed so that these nodes in the same contact elements are on the same partitions, or PEs. Table 4 shows the results obtained by this partitioning method. The number of iterations for convergence has been dramatically reduced for each preconditioing method. In the $\lambda = 10^{10}$ case, CG with SB-BIC(0) converges in a reasonable number of iterations, although BIC(2) stagnates, even with the new partitioning method.

Table 2. Iterations/CPU time (includes factorization) until convergence ($\varepsilon = 10^{-8}$) on a 4 PE COMPAQ Alpha 21164/600MHz cluster using CG with block preconditioning for the 3D elastic fault-zone contact problem in Figure1 (21,660 DOFs). **(ORIGINAL partitioning)**

Preconditioning	λ	Iter #	sec.
BIC(1)	10^0	44	4.1
	10^6	1,724	70.7
BIC(2)	10^0	86	6.6
	10^6	962	59.8
	10^{10}	NO. Conv.	N/A
SB-BIC(0)	10^0	156	3.5
	10^6	1,598	33.9
	10^{10}	2,345	55.5

Table 3. Iterations/CPU time (includes factorization) until convergence ($\varepsilon = 10^{-8}$) on a 4 PE COMPAQ Alpha 21164/600MHz cluster using CG with block preconditioning for the 3D elastic fault-zone contact problem in Figure1 (21,660 DOFs). **(IMPROVED partitioning)**

Preconditioning	λ	Iter #	sec.
BIC(1)	10^0	80	3.8
	10^6	167	7.4
BIC(2)	10^0	71	5.8
	10^6	74	5.9
	10^{10}	NO. Conv.	N/A
SB-BIC(0)	10^0	126	2.9
	10^6	124	2.8
	10^{10}	231	5.7

4. Large Scale Computation

Efficiency and robustness of the developed preconditioning and partitioning methods for simulations of fault-zone contact has been evaluated in 3D large-scale applications on parallel computers. Simple geometry and boundary conditions of an example model for 3D, linear elastic solid mechanics were considered. In this example, linear multiple point constraint (MPC) conditions have been applied to the nodes in contact groups. The problem and boundary conditions are as follows:

- Three zones with uniform material property with non-dimensional E (Young's modulus)=1.0, ν (Poisson ration)=0.30.
- Uniform MPC conditions have been imposed on the nodes along the boundary surfaces of the blocks.

A large-scale computation (total elements=784,000, total nodes =823,813 and total DOF=2,471,439) was performed on the example model. This example was solved by parallel iterative solvers with various types of preconditioning methods under various penalty numbers for the MPC conditions. The problem is linear elastic and the coefficient matrix is symmetric, therefore the CG method was adopted. Domains are partitioned according to the contact group information described in the previous chapter. Computations were done with 128 PEs on a Hitachi SR2201 at the University of Tokyo.

Table 4 shows the results for various combinations of preconditioning methods. SB-BIC(0) preconditioing is more efficient and robust than other methods such as BIC(0), BIC(1) and BIC(2). BIC(0), BIC(1) and BIC(2) become unstable and the number of iterations for convergence increases as the penalty number λ increases. In contrast, the number of iterations for convergence for SB-BIC(0) remains constant while λ increases.

Table 4. Iterations/CPU time (includes factorization) until convergence ($\varepsilon = 10^{-8}$) on a 128 PE Hitachi SR2201 using preconditioned CG for the 3D elastic contact problem with MPC condition (2,471,439 DOF). Contact group information is considered.

Preconditioning	λ	Iter #	sec.
BIC(0)	10^2	905	194.5
	10^6	>8,300	>1,800.0
BIC(1)	10^2	225	92.5
	10^6	297	115.2
	10^{10}	460	165.6
BIC(2)	10^2	183	139.3
	10^6	201	146.3
	10^{10}	296	187.7
SB-BIC(0)	10^2	542	69.5
	10^6	542	69.5
	10^8	543	69.7
	10^{10}	544	69.8

5. Conclusions and Further Study

In this study, robust preconditioning and partitioning methods were developed for the simulation of fault-zone contact with penalty constraints using parallel computers. For symmetric matrices, block incomplete Cholesky factorization without inter-block fill-in, using *selective blocking* (SB-BIC(0)) shows excellent performance, memory efficiency and robustness. SB-BIC(0) remains stable for a wide range of penalty number values, while the performance of BIC(1) or BIC(2) declines according to the penalty number. It is also shown that the partitioning method for elimination of edge-cuts in contact groups improves convergence of parallel iterative solvers with localized preconditioning.

In the next stage, we are implementing these newly developed preconditioning methods into the linear solvers of the GeoFEM platform and are going to solve larger-scale, realistic contact problems with friction using many processors. In this study, infinitesimal, linear elastic deformation theory was assumed, although in real simulations we have to consider large slip and large deformation, where node location and the connectivity of contact groups can dynamically change. More robust preconditioning method and dynamic

Acknowledgments

This study is a part of *the Solid Earth Platform for Large-Scale Computation* project funded by the Ministry of Education, Culture, Sports, Science and Technology, Japan through *Special Promoting Funds of Science & Technology*. Furthermore the authors would like to thank Professor Yasumasa Kanada (Information Technology Center, University of Tokyo) for fruitful discussions on high performance computing and Dr. Tomoshi Miyamura (Nihon University) and Mr. Mikio Iizuka (RIST) for discussions and suggestions on simulations of fault contact.

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